The compound crystallizes in the space group $P2_1/c$ with a = 9.922(2), b = 8.462(2), c = 16.068(2) Å, β = 100.29(1)°, D_m = 1.208 gm/cm^3, D_c = 1.197 gm/cm^3, μ(CuKα) = 6.175 cm^{-1} and Z = 4. The structure was solved by MULTAN with 1705 unique reflections collected on a diffractometer. 170 reflections with E_{max} = 4.549 and E_{min} = 1.682 were used to solve the phase problem and all the non-hydrogen atoms were shown by the search map of MULTAN. The positional and thermal parameters of non-hydrogen atoms were initially refined by full-matrix least square method. A difference map at R = 0.12 revealed some of the hydrogen atoms and the rest were generated. They were assigned isotropic temperature factors of non-hydrogen atoms to which they were attached. The positional parameters of hydrogen and non-hydrogen atoms and their isotropic and anisotropic thermal parameters respectively were refined by block diagonal least square method and the final R-value was 0.0432. The bond lengths and angles were well within the range of chemically accepted values and the non-bonded contacts were always greater than the sum of the Vander Waals radii.

The derived three-dimensional molecular architecture confirms the stereospecificity of the reduction process and the formation of a CIS Ketone. The ring fusion methyl group is axial to the B-ring and equatorial to the Ketone containing A-ring of the molecule, whereas the ring fusion hydrogen atom is equatorial to the B-ring and axial to the A-ring of the molecule. The estimated distance between the hydrogen atom attached to C_4 and the hydrogen atom attached to C_5 of the aromatic benzene ring reveals that the alternative conformer with the methyl group equatorial to B-ring and the hydrogen axial to it is not favoured in the crystalline state.

09.2–7 CRYSTAL AND MOLECULAR STRUCTURE OF 2-METHYL-1,2,3,9,10,10a-HEXAHYDRO-2α,10aα,11-OXOETHANOPHENANTHRENE. By A.K. Pal*, S.C. Kundadas and B.S. Basak, X-ray Laboratory, Presidency College, Calcutta-73, India.

The title compound ($C_{17}H_{18}O$) is one of a number of important organic compounds studied in our laboratory. The compound crystallized in space group $P2_1/c$, a = 10.109(4), b = 11.725(5), c = 11.159(1)Å, β = 94.24(5)°, V = 1319Å^3, D_c = 1.20 g cm^{-3} for Z = 4, D_m = 1.18 g cm^{-3}, F(000) = 512, μ(MoKα) = 0.78 cm^{-1}, λ(MoKα) = 0.7107Å.

Three-dimensional diffraction data were recorded on a four-circle diffractometer by ω-2θ scans. A total of 2314 reflections were collected, including 1058 with $|F_o| \leq 4\sigma(F_o)$. The structure was solved by direct methods using the 1978 version of MULTAN. The structure was refined isotropically and also anisotropically using the program MAMIE for full-matrix least-squares and the program BLOK for block-diagonal least-squares calculations, respectively. Prior to anisotropic refinement, the positions of the hydrogen atoms were determined by difference synthesis. The refinement ended with R = 0.048.

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09.2–8 CRYSTAL AND MOLECULAR STRUCTURE OF cis-METHYL-3,4,4a,9,10,10a-HEXAHYDROPHENANTHRENE-2(1H)-ONE-4a-ACETATE.
By A.K. Pal*, S.C. Kundadas and B.S. Basak, X-ray Laboratory, Presidency College, Calcutta-73, India.

The crystal structure analysis of the title compound is part of a structural study of biologically important organic compounds. The compound ($C_{17}H_{20}O_3$) crystallised in space group $P\bar{1}$, a = 6.413(1), b = 10.501(3), c = 10.862(4) Å, α = 82.71(2), β = 87.73(2), γ = 85.29(2)°, V = 724Å^3, D_c = 1.24 g cm^{-3} for Z = 2, D_m = 1.23 g cm^{-3}, F(000) = 584, μ(MoKα) = 0.91 cm^{-1}, λ(MoKα) = 0.7107Å. Three-dimensional counter data were recorded using ω-2θ scans. A total of 1880 reflections were measured, including 944 with $|F_o| \leq 4\sigma(F_o)$. The structure was solved by direct method using the 1978 version of MULTAN. It was refined first isotropically and then anisotropically using the programs MAMIE and BLOK for full-matrix least-squares and block-diagonal least-squares calculations, respectively. The hydrogen atoms were located prior to the anisotropic refinement. The refinement converged with R = 0.055.

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09.2–9 CRYSTAL AND MOLECULAR STRUCTURE OF 6-(3-HYDROXY-3-METHYL-1-BUTINYL)-7-METHOXY-2H-1-BENZOPYRAN-2-ONE (SUBERINOL).
By R.R. Bandyopadhyay* and B.S. Basak, X-ray Laboratory, Presidency College, Calcutta-700073, India.

The crystal structure of suberinol ($C_{15}H_{16}O_4$) has been determined as part of a study of the structures of biologically important organic compounds. Suberinol crystallized in space group $P2_1/c$, a = 7.94, b = 15.64, c = 10.99Å, β = 103.97°, V = 1324Å^3, D_c = 1.30 g cm^{-3} for Z = 4, D_m = 1.29 g cm^{-3}, F(000) = 552, μ(CuKα) = 7.87 cm^{-1}, λ(CuKα) = 1.5418Å. Three-dimensional X-ray diffraction data (OKℓ to 6kℓ, h0ℓ, hlℓ) were recorded photographically using a Unicam Weissenberg goniometer. The structure was solved by direct methods. Isotropic followed by anisotropic refinement calculations were made by means of the full-matrix least-squares program MAMIE and the block-diagonal least-squares program BLOK, respectively. The final R = 0.09. Bond lengths and bond angles agree with the values in similar compounds.

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